

Study of the structure of 1-nitro-3,3,3-trifluoro- and 1-nitro-3,3,3-tribromopropenes by the methods of dipole moments and quantum chemistry

Vereshchagina Y., Alimova A., Chachkov D., Ishmaeva E., Slobodchikova E., Berestovitskaya V.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2014 Pleiades Publishing, Ltd. Method of dipole moments and quantum-chemical calculations allowed establishing that 1-nitro-3,3,3-trifluoro- and 1-nitro-3,3,3-tribromopropenes have the E-configuration (the nitro group and the trihalomethyl substituent are in the trans-position); the obtained characteristics were compared with the corresponding data for the trichloromethyl-containing analog.

<http://dx.doi.org/10.1134/S1070428014110049>
